

Isopropanol

67-63-0 | DTXSID7020762

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -99.6 °C

Global applicability domain: Inside

Local applicability domain index: 7.95e-01

Confidence level: 5.82e-01

Nearest Neighbors from the Training Set

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Isopropanol

Measured: -89.5

Predicted: -99.6

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1-Propanol

Measured: -126

Predicted: -114

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2-Methyl-1-propanol

Measured: -108

Predicted: -103

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1-Butanol

Measured: -89.8

Predicted: -95.0

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2-Butanol

Measured: -115

Predicted: -70.5